

Simulation Platform for Multiscale and Multiphysics Modeling of OLEDs

M.Bogdanova^{1*}, S.Belousov^{1*}, I.Valuev^{1,4*}, A.Zakirov¹, M.Okun¹,
D.Shirabaykin¹, V.Chorkov¹, P.Tokar¹, A. Knizhnik¹, B.Potapkin¹,
A.Bagaturyants^{2,3}, K.Komarova^{2,3}, M.N.Strikhanov³, A.A.Tishchenko³,
V.R.Nikitenko³, V.M.Sukharev³, N.A.Sannikova³, I.V.Morozov⁴

¹ Kintech Lab, Moscow, Russia

² Photochemistry Center of the Russian Academy of Sciences (PC RAS), Moscow, Russia

³ National Research Nuclear University «MEPhI», Moscow, Russia

⁴ Joint Institute for High Temperatures of the Russian Academy of Sciences, Moscow, Russia

bogdanova@kintechlab.com, belousov@kintechlab.com, valuev@kintechlab.com

Abstract

We present a simulation platform which serves as an integrated framework for multiscale and multiphysics modeling of Organic Light Emitting Diodes (OLEDs) and their components. The platform is aimed at the designers of OLEDs with various areas of expertise ranging from the fundamental theory to the manufacturing technology. The platform integrates an extendable set of in-house and third-party computational programs that are used for predictive modeling of the OLED parameters important for device performance. These computational tools describe properties of atomistic, mesoscale and macroscopic levels. The platform automates data exchange between these description levels and allows one to build simulation workflows and manage remote task execution. The integrated database provides data exchange and storage for the calculated and experimental results.

Keywords: organic light emitting diodes, simulation platform, multiscale multiphysics simulation, distributed computing, quantum chemistry, drift-diffusion, FDTD, ray-tracing

1 Introduction

Organic light emitting diodes (OLEDs) are flat and thin large-area light sources that form a branch in the technology of solid state lighting which has been actively developing over the last decade. The working principle of OLEDs is based on the electroluminescence - the radiative recombination of injected electron-hole pairs in a solid, which is fundamentally different from thus far existing lighting techniques and holds the promise for highly efficient, long-lived, and environmental friendly light

* Corresponding authors

sources (1). Modeling of light outcoupling and efficiency of OLEDs is a very complex physical problem. From the optical point of view the outcoupling of light emission in an inner layer of a planar multilayer structure could not be higher than 20% (2). The electrical charge transport in organic structure depends strongly on layer energy properties and geometry of a device (3). Microstructure of the organic layer defines the energy properties of transport levels and depends on the synthesis conditions of the material. The properties of a fluorescent molecule in a specific surrounding define the fluorescent spectrum and power.

Each of the described above processes is simulated by a corresponding numerical method. Finite different time domain (FDTD) (4), ray tracing and transfer matrix (5) methods deal with the optical aspects. Monte-Carlo method and drift-diffusion simulations describe the charge transport in organic media. With molecular dynamics methods it is possible to obtain the layer bulk or interface microstructure either for polymers or for small molecule systems. Quantum chemistry deals with the spectrum and energy of a single molecule playing a role of recombination or charge transfer site.

The output data from each spatial (and consequently physical) level that is considered in our simulation platform is used as the input for the next level. The typical compute time and resources for each of the methods are very different. Because of this we employed distributed computing and workflow/data management to execute compute scenarios required for simulation of OLED physics and optimization of device parameters. The platform includes a number of numerical models in each physical level (calculation modules), task manager (calculation scheduler), data storage system and database, graphical user interface.

The platform implements a well-developed “Scientific workflow” concept. It has an open architecture: the user can add, modify and replace calculation modules without developers. It supports multiuser collaboration and data exchange and provides highly performance, scalability and flexibility in customization and configuring.

In our platform we use a set in-house (developed in Kintech Lab and MEPhI) simulation codes and provide interface to several third party codes. The third party codes are not distributed with the platform and should be individually obtained and installed by the users. The list of the software currently interfaced by the simulation platform contains the following programs: GAMESS (US) (6), Quantum Espresso (7), MD-kMC (developed in Kintech Lab, Moscow, Russia) (8), GROMACS (9), Monte-Carlo simulation of hopping transport (developed in MEPhI, Moscow, Russia), FDTD-II (based on EMTL, developed in Kintech Lab, Moscow, Russia) (10), Ray Tracing code (based on EMTL, developed in Kintech Lab, Moscow, Russia) (11), T-matrix code (based on the CAMFR program) (12), Drift-Diffusion code (developed in Kintech Lab, Moscow, Russia).

2 Related Work

The modern approaches of numerical simulation of OLEDs include both well-developed methods and new techniques. For optical modeling one has successfully applied the finite-difference time domain method (see Section 3), finite element method (13), ray tracing (14) and other computational techniques. Special organic-material versions of Monte-Carlo method (15) and drift-diffusion (16) were used to describe the charge carrier transport. The possibilities of the integrated into the platform physical models take the up to date state of the OLED research into account and are described in Section 3.

There exist several software tools that are dedicated to simulation of OLEDs. Examples are SetFos by FLUXIM AG and SimOLED by Sim4Tec Ltd. These programs are specialized device-oriented software dealing with the optical and charge carrier transport level of the OLED simulation. Our platform is different from these tools mainly because it is designed to possibly cover the whole area of the related physics from atomistics up to the device properties. Rather than being a single specialized

program it combines different calculation programs and methods that may originate from various research groups or be commercial software.

On the other hand, there exists a variety of scientific workflow platforms and tools such as Kepler, Taverna, MAPPER, Triana, Pegasus. Generally these tools are universal and allow one to build a scientific workflow from a set of calculation routines and to execute this workflow using existing compute resources. Usually the prerequisite for these tools is an infrastructure of some kind: there must be either a functional Grid environment or web portal, most of the tools require Condor software to manage the task execution. Although it is possible to use a universal tool to build a research-specific distributed simulation framework, we found the requirements to maintain the Grid infrastructure, user registration and the limitations of the interface too restrictive for the needs of OLED simulation. Instead we followed a route of creating a relatively lightweight application that can be installed even on a single computer and that can operate remote compute resources in a passive way on behalf of the user. For the purpose of task and workflow management we used a free C++ library called GridMD (17), which is able to communicate with various task scheduling systems, including Globus Grid (see Section 4.2).

Another significant feature of our approach is the data specialization, which was performed for the OLED area. Instead of operating the universal data entities such as files or numbers on a user level (which most workflow systems do), the user is offered to work with structured data types that have physical meaning for the OLED scope (see Section 4.1). Certainly, these data types may be extended, and new types added, but these software configuration procedures are hidden from the standard user. Thus being a physicist or a technologist, the standard user is not required to have an expert level in software configuration and scripting.

3 Physical Models

Numerical simulation tools include three spatial scales: atomistic scale deals with the molecular properties, mesoscopic scale deals with the energy and structure properties of a single layer, macro (device) scale deals with the optical and electrical properties of a multilayered device. In the following subsections we briefly describe the utilized physical models and the computational resources required by the simulation tools.

3.1 Atomistic Level

The platform integrates two levels of atomistic scale simulations. They are presented as a specialized GUI and data exchange scripts which support the following third-party products:

1. GAMESS (US) - a general ab initio quantum chemistry package, which is maintained by the members of the Gordon research group at Iowa State University (6);
2. Quantum Espresso - an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale (7);
3. GROMACS - a versatile package to perform molecular dynamics, i.e. simulate the Newtonian equations of motion for systems with hundreds to millions of particles (9).

We use also one of our in-house programs for molecular dynamic calculation of polymer materials:

4. MD-kMC (molecular dynamics method) allows calculating the geometry of polymer layer microstructure (8).

The first level includes the simulation of the photophysical properties of a single molecule in specific media. The GUI is designed to configure several types of calculations: emission spectra and

radiation lifetime simulation, including the effect of spin-orbit coupling between singlet and triplet states; excited state energies calculation; distribution function simulation for HOMO and LUMO energies in a layer; reorganization energy calculation; metal work function calculation based on density-functional theory, plane waves, and pseudopotentials.

All these calculations use the density functional theory with hybrid or coulomb-attenuated functionals, which provides fast and good quality simulations both for exciton and charge-transfer characteristics. The distribution function calculation for HOMO-LUMO energies requires the microstructure of small molecules bulk as an input. It is calculated using molecular dynamics simulation.

The second level provides insight into molecular packing in a layer within molecular dynamics approach. The molecular structure of the layer, average distance between molecules and layer density could be simulated. Three tasks are implemented: small molecules bulk simulation; polymer molecules bulk simulation; simulation of the interface between two layers.

Quantum chemistry calculations are limiting the overall performance of the atomistic level scenarios. The total computational time to calculate atomistic properties can be rather long (up to one week for a single run on a supercomputer). However the material properties which can be obtained with these runs could be used in various macroscopic simulations without being recalculated again. These material properties may be stored in a database which we developed especially for this project. In the subsequent optical and electrical calculations either experimental or calculated material properties could be used.

3.2 Mesoscopic Level

Monte-Carlo Simulations for Mobility and Diffusion Coefficients.

Hopping charge transport, energetic (diagonal) and non-diagonal (spatial) disorder are the inherent features of organic materials. Hopping rates are distributed randomly and vary by many orders of magnitude from site to site. Modeling of mobility and diffusion coefficient, hence, requires calculations on the mesoscopic scale, which exceeds considerably mean inter-molecular distance. Monte-Carlo (MC) simulations, although time-consuming, seem to be the most adequate modeling tool for disordered organics. Therefore, MC-modeling of charge transport in separate organic layers has been integrated into the developed simulation platform.

Disordered organics is modeled by a cubic lattice with site energies, distributed randomly in accordance with the Gaussian law. One can consider only a fraction of lattice sites as hopping centers, in order to model non-diagonal disorder. Charge carrier, being born at injecting electrode, has to perform random walk across a layer, which is biased by a given voltage. The algorithm of MC-modeling of the random walk is standard and has been described previously (18). Charge carriers are generated at a given concentration at the injecting electrode, and the calculation proceeds until a stationary concentration establishes inside the entire sample.

The modeled quantities are the charge current density across every layer of hopping centers, the local concentration of charge carriers and the local electric field strength (the latter is related to the charge density via Poisson's equation). The local mobility and diffusion coefficients are extracted from the equations for current density at two adjacent layers. This procedure yields the field- and concentration-dependent mobility and diffusion coefficient for a given organic layer.

Site hopping Monte-Carlo simulation is implemented as a parallel program which is well scaled with the number of CPUs and requires typically up to 100 CPU-hours to execute.

3.3 Device Level

Drift-Diffusion Method for Charge Carrier and Exciton Transport and Kinetics

On the continuous medium scale the charge carrier transport and exciton dynamics is represented in the platform by the drift-diffusion model and the corresponding numerical tool developed at Kintech Lab. The organic nature of the layer materials is manifest in site energy disorder (Extended Gaussian Energy Disorder (EGDM) (19)) and generalized Einstein relation between the charge mobility and diffusion coefficients (20). The dependence of the mobility on the field strength and carrier density could be modeled either with the Pool-Frenkel function or with EGDM relations. The code includes reflected charge model for a contact with metals.

Each material is characterized by a set of parameters: charge carrier mobility model and its constants, HOMO and LUMO levels, disorder parameter, density of states for charges, kinetic coefficients for exciton dynamics. Some of these material parameters may be obtained from the experimental literature; however most of them cannot be measured directly and fitting procedures are required to extract the parameter values. Our platform has an advantage of calculating the material properties (or at, least, many of them) in an ab-initio way from the atomistic models. As a result of charge transport simulations the electrical properties of a device can be obtained: the current-voltage curve, distribution of the charge concentration within a device, distribution of the exciton concentration in the emissive layer.

The most essential computation operation in the drift-diffusion code is the sparse matrix inversion in course of the Newton-Raphson iteration procedure. For the 1D model which is generally sufficient for the OLED emissive layer description, the drift-diffusion code requires less than 1 CPU-hour to calculate the whole current voltage curve. The model is implemented as a sequential code that can be run locally or remotely.

Optical Properties

Modeling of optical properties of an OLED is a crucial step in evaluation of the overall device efficiency (2) (1). The optical simulation provides information about OLED optical performance in terms of the total emitted power, outcoupled power and angular pattern as functions of the wavelength of the emitted light. Optical performance of an OLED depends on several factors: its geometry, material properties of constituent layers, the position of the emitting region within the OLED. The latter is dependent on the charge transport properties of the device and should be input from the charge transport simulations.

OLED geometry is the key to optimizing optical performance of the device. Strong enhancement of the optical performance can be achieved by applying either one of several approaches, such as varying the thickness of layers (21), adding specific geometric features at different scales, such as periodic or random corrugation of the interfaces (nanoscale) (22) (23) (24), introducing volumetric scattering layers (microscale) (25), modifying the substrate with microlenses (micro- and macroscale) (26), or combination thereof. Essentially, the OLED consists of a stack of thin layers where emission occurs (overall thickness of the order of the emitted light wavelength) and several thick layers including the substrate (thickness is much greater than the wavelength of emitted light). Therefore optical modeling of OLEDs can be naturally split in two parts:

1. Full-wave calculation of electro-magnetic field propagation in the thin layers. In this calculation, the first adjacent thick layer (e.g. substrate) is considered semi-infinite. The outcoupled power and angular pattern in the first adjacent thick layer are the outputs to be calculated.
2. Geometrical optics calculation for the rays propagating in the micro- or macrostructured layers (substrate, volumetric scattering layers). The angular pattern from the full-wave calculation serves as an input to this calculation. Ultimately, both the outcoupled power and angular pattern in the air are obtained.

In our platform the full-wave calculation may be combined with the geometric optics to perform a through-out optical characterization of OLEDs on nano and micro / macro scales. Optical modules in

the platform incorporate several methods and predefined workflows optimized for modeling of different geometries. Full-wave calculation for thin layers includes:

1. Semi-analytic transfer matrix approach (TM) is used for calculating the properties of a planar OLED. The emitter is treated as a dipole source, the problem is essentially one-dimensional, that is, only the position of the dipole with respect to the layer interfaces is used as an input for the calculation. The total emitted power, outcoupled power and angular distributions are simultaneously calculated for dipoles oriented both parallel and normal to the layer interfaces. Averaging over the dipole orientations is performed (5).
2. Finite-difference time-domain method (FDTD) (4) is used for calculating the properties of OLEDs with corrugated interfaces, where the simple planar approach is not applicable. The emitter is treated as a dipole source, the dipole source position with respect to the layer interfaces as well as the corrugation features are used as inputs. Each calculation deals with a certain dipole position and orientation. The total emitted power, outcoupled power and angular distributions are calculated. Averaging over dipole orientations and essential positions with respect to the corrugation features is performed.

Geometric optics is realized with ray-tracing method (RT) (14). This method is used for calculating the propagation of rays in the thick layers. The angular pattern of the radiation from the thin layers (obtained by the full-wave calculation) serves as an input to the RT model. Different types of scattering behavior are incorporated in the model: Fresnel reflection / refraction at smooth media interfaces; Mie scattering on randomly distributed particles (volumetric scattering); back reflection from the thin layer stack is calculated with the transfer-matrix approach. In the ray-tracing calculation, reflection of light from the thin layers of OLED is calculated with the T-matrix formalism (27). Ultimately, ray-tracing calculation yields bidirectional scattering function (BDSF) of thick layer as well as the angular pattern of radiation of OLED in the surrounding medium (air). Both the outcoupled power and angular pattern in the air are obtained.

The used optical models have various computational resource requirements. The most resource consuming model is the full wave FDTD method. There are several aspects, which determine the time and memory resources needed to obtain a reliable result with this method. Firstly, transverse dimensions of the modeled OLED should be sufficiently large in order to avoid edge effects. The transverse size is generally determined by the attenuation length of surface waves, excited by a source in thin layers of the OLED. The typical lateral dimensions are 20 by 20 microns and can be larger depending on the materials used. Secondly, the spatial mesh resolution should be sufficiently small in order to accurately account for large field gradients in the nano-structured device. The typical mesh step is then less than 5 nm. These considerations put memory requirements of FDTD at 100-200 Gb for the modest estimation, whereas the typical single run simulation is 500-800 CPU-hours. Moreover, several dipole orientations and positions in the nano-structured OLED should be separately evaluated in order to fully characterize its optical properties. Typically, the number of such runs amounts to ~10. We use the scalable FDTD implementation that is based on EMTL library, which allows for effective employment of large HPC systems for the FDTD runs.

The semi-analytical TM method is not time-consuming and is implemented as a serial code. Compute resources required by a ray-tracing calculation depend largely on the number of rays launched. In a typical calculation, the number of rays is $\sim 10^7 - 10^8$, and a typical run requires around 1 CPU-hour. We implement the ray tracing model on the base of the EMTL geometrical primitives and use a perfectly scalable MPI version to run on an HPC system.

4 Simulation Platform Architecture

The architecture of the developed platform is outlined in Figure 1. The platform consists of a set of modules that are managed from the executable running on a client machine. The manager application provides platform operation and data transfer. Some platform modules are part of the manager program and some are external programs. The manager application and all client modules are cross-platform and have Windows and Linux versions. The platform includes graphical user interface modules, calculation modules, business logic modules, database of materials properties and structures and the result storage system. The modules are interacting with each other by the standard communication protocols. All platform modules can be divided into 3 levels (columns from left to right in Figure 1):

GUI level – provides interaction with the user, data input and visualization;

Data storage level – provides initial data and calculation results storage along with access to this data from GUI and business logic modules;

Calculation level – provides calculation modules management

This multicomponent platform architecture ensures platform scalability and possibility of relatively simple module replacement.

4.1 Platform Data Exchange

The core parts of the simulation platform making it suitable for multiscale multiphysics simulation are data storage system and data exchange module. They combine simulation tools operating on different physical scales in one calculation project. The key concept of the data exchange system is a data type, which is a structure of primitive data fields such as numbers, tables, character strings. The data types that are available in the project reflect the physical specifics of the OLED research. There are several tens of the defined data types for transferring material properties, model parameters and calculation results. Since each field of the data type has its physical meaning, the visualization or editing tools may be associated with certain data types. Also the data of a defined type is used to fill input and output ports when the computational modules are operated on the GUI desktop.

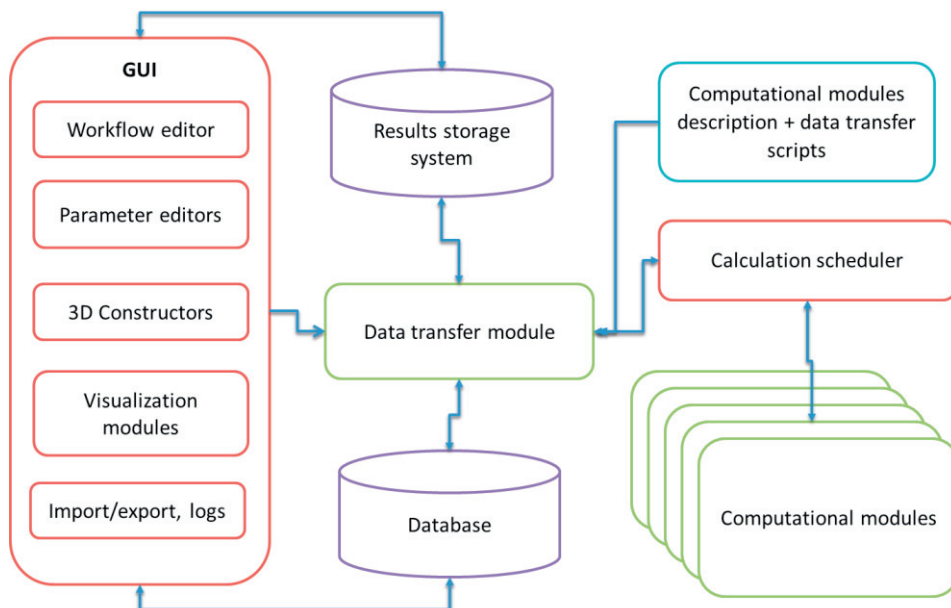


Figure 1 Multiscale platform architecture

Each project has an associated data storage, where the structured (typed) data is placed after finishing of each calculation tool and from where it is retrieved for constructing the input to the next calculation tool in the workflow chain. For example, the atomistic level models (quantum chemistry), meso-scale models (molecular dynamics) and device-scale models (FDTD, Ray tracing, etc.) are connected in our platform with the help of suitable data exchange procedures, extracting the typed data from the calculation outputs (data import) and constructing the application specific input files (data export). Only the data important for the purpose of the calculation module in the OLED-specific computation is extracted this way, so this stage assumes some area-specific filtering of the output. These procedures (data transfer scripts) are included in the workflow as auxiliary tasks and become part of the simulation scenario.

Data exchange module implements a data storage for the calculation project, where all calculation results and calculation modules parameters are stored in a structured way in the xml format. Thus despite of the fact that the platform architecture and the main platform components are universal, the project data file is application-specific. All the data used in calculation are divided into physically important categories grouped in “ports”. The ports can contain input or output of the calculation module and some specific parameters such as project status, links to files with results, etc. (Figure 2).

Data exchange module is a script-based data conversion engine. It operates in two regimes

- extracting important data from calculation results files and saving this data to project data storage;
- template-based generation of the input files for calculation models based on the data from project data file.

Data conversion scripts are written in Java Script language. These scripts are created for each integrated third-party computational program, while the in-house computational tools are usually programmed to understand the project file XML format and do not require conversion scripts. These scripts can be modified by the user without requirement to modify or recompile the other platform components. This constitutes also the mechanism for third party or user-developed simulation tools adaptation for the simulation platform. When adapting a new module the corresponding data exchange scripts should be created while following certain documented specifications on data types. As mentioned in the preceding sections, the physical properties significant for the OLED model are grouped in data types. New data types may be added as necessary when including new modules, making the corresponding new data ports available for data exchange in the workflow.

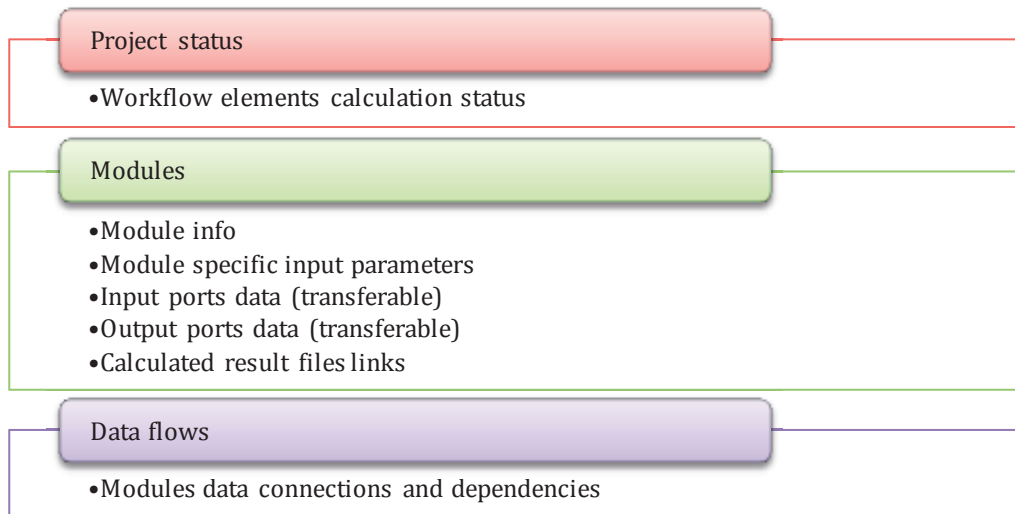


Figure 2 Project file structure

4.2 Calculation Task Management

Scenarios created by the user of the simulation platform with the help of the graphical user interface describe mainly the physical problem to be solved and the corresponding data flow between coarse-level modules. These modules may in turn contain lower level computational tasks, which exact composition and execution sequence is hidden from the user. For example, each module represented as an icon on the desktop may imply a sequence of runs of different applications with data transfers between them. These applications may include actual computational programs and also auxiliary tools such as data converters. The low-level workflow resulting from a combination of subtasks for the whole scenario specified by the user is created automatically by the business logic modules when the user starts calculation. As well as the data exchange scripts, the scenarios specific to a certain calculation module may be configured or modified by an expert user.

The description of the project workflow is passed to a special component called task manager. Task manager schedules the tasks on the corresponding computational resources, collects and passes data between tasks and maintains the status information on the whole computation.

Task manager is created on the base of GridMD workflow library (17). Originally this library was designed for programmers of (molecular dynamics) compute applications allowing for distributed execution. GridMD is a lightweight portable C++ library, that contains universal APIs for access to remote systems using SSH, scheduling compute jobs with different cluster queue managers (PBS, SLURM, Linux/Windows command shells) as well as Grid environments. Job management in GridMD is organized in the passive mode, not requiring any task management agents or special programs to be running or even installed on the remote system. The workflow execution is monitored by a tool (task manager) running on a client machine and authorizing itself on remote compute sites with the user credentials. Apart from standard local or remote application launches, GridMD workflow may also manage tasks that are described as a local code (compiled as part of task manager) executed on the client. Moreover, these local tasks may change the workflow dynamically by adding additional jobs or dependencies to the existing workflow graph. This feature simplifies auxiliary processing for a programmer: it is possible to put all task management procedures into a single portable C++ code. Data transfer between different compute resources and from the client machine and a compute resource is performed via the exchange of files. Task manager is able to checkpoint and restart the whole workflow, to recover from different types of errors that can happen while executing applications. Task manager can easily be terminated on the client machine, for example when the user exits the simulation platform GUI. The workflow in this case can be restored and continued when task manager starts again.

5 Graphical User Interface

The platform graphical user interface (GUI) is a client program operated by a user. The GUI program has Linux and Windows versions and may be generally run on any local machine. The GUI is used to operate calculation modules, initialize data, create workflows, manage the calculation process and analyze results.

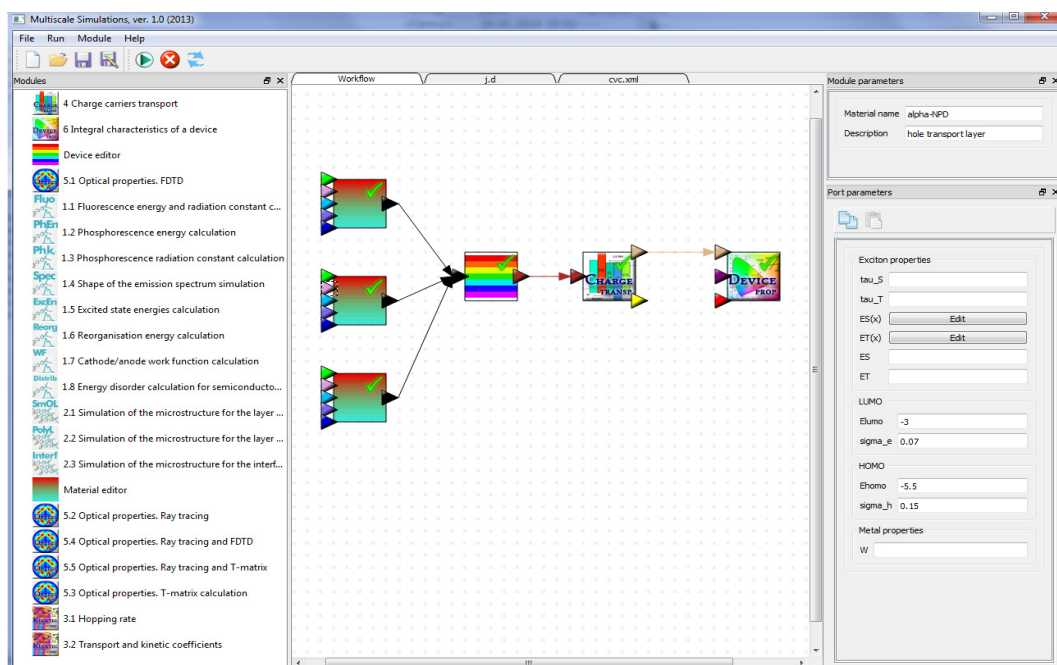


Figure 3 Multiscale platform: main window

The main window of the platform GUI is separated into three areas: the list of calculation modules (left side of Figure 3); the desktop («Workflow» insert) (in the middle of Figure 3) and the panel of calculation parameters (the right side of Figure 3). The user can construct a calculation workflow by dropping the calculation modules and editors from the list on the left and connecting them by arrows. Each arrow means an automatic data transfer from one calculation module to another.

The right hand panel appears when the user selects one of the module icons on the desktop by a mouse click and contains two parts: “Module parameters” and “Port parameters”. The “Module parameters” subpanel may contain several inserts with the input data for all numerical models which are used in the selected computational module. All parameters in this part of the window are model-specific and they could not be a result of any previous calculation. Examples of such model-specific settings are mesh sizes, the number of iterations, and residue maximum for the drift-diffusion module.

The “Port parameters” subpanel also contains inputs for the calculation; however they may be (but not necessarily) obtained as an output from another calculation module. These data are called the transferable data and may be used for specification of the workflow. The transferable data is grouped into so-called ports according to the physical meaning for the OLED simulation. The ports may be used to connect modules on the desktop and are marked by the colored triangles on the module icons. Each color corresponds to a particular data type. In the case when an input port of one module is connected with an output of another one the data will be transferred automatically as soon as the calculation of the first module is complete. If there are no workflow connections an input port can be filled in “by hands” by editing the data fields in the “Port parameters” panel. If the connection exists the port data can also be viewed after the calculations performed by the previous module.

Each computational module generates outputs of two types: transferable and non-transferable results. Transferable results can be used as input for the next module in the chain and therefore are sent to the output port; non-transferable but useful results appear in the Module/Results drop-down menu. These results may be viewed in GUI in various ways, for example as a text or as a graph/picture.

6 Integrated Database

The OLED simulation platform is supplied together with the application-specific database which is intended for storage of some finished results or experimental data that may be important in other calculations or have to be shared by a group of researchers. Thus the database is not directly used for the data exchange between modules, but rather for the results and model parameters exchange for the platform users. The database contains atomistic, transport and optical properties of the materials that are relevant for OLEDs. These properties are obtained either from the experimental data and literature, or from numerical simulations, and can be efficiently used for subsequent modeling and development of OLEDs. From one side, the database is a warehouse for storing data, and from the other side it is the source of the data to use as an input for calculation modules.

The database is based on free portable SQL server Firebird 2.5, formerly known as Interbase. It is developed by the open source community and has versions for various operating systems: Windows, Linux, MAC. The main features of the database include:

- Client-server architecture – possibility to use centralized database server for project group or laboratory along with the local user database;
- Multiuser access to the database with user rights management;
- Data tracking and database change log system. Generation of reports with database modification history;
- Portability – the same code works under a variety of operation systems.

7 Example of Calculation

In Figure 4 we present the workflow for calculation of a single carrier device electrical properties. This computational chain aims to obtain the energy parameters of charge carriers in an organic material and then to calculate the voltage-current characteristic for a single layer device (organic layer between two electrodes).

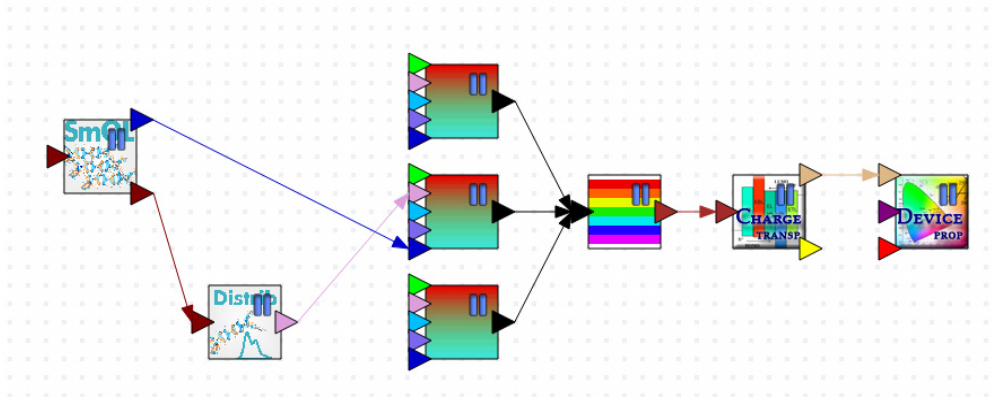


Figure 4 Example of multilevel calculation of a single carrier device electrical properties

Two computational modules on the atomistic scale are involved: the module for calculation of microstructure for small molecule organic layer (the first unit in the chain), the module for calculation of energy disorder in semiconductors (second unit in the chain).

In a single layer device there are three different materials: anode, cathode and organic layer. Each material is represented by an icon on the desktop. The parameters of metals (the anode and cathode) in this calculation are taken from the literature and are filled in the input port parameters manually. The

material properties of an organic layer are being calculated with the atomistic modules mentioned in Section 3. We obtain the density of states for charge carriers directly from the molecular dynamics calculation (blue arrow), the energy and disorder parameters of HOMO and LUMO levels (rose arrow) are the result of the quantum chemistry calculation with the layer microstructure (dark brown arrow) obtained from the molecular dynamics. The material parameters (black arrows) are collected in the device geometry module (the third one from the right in the chain). This unit allows constructing the device with any number of layers with complex geometry. Then the constructed geometry with material parameters (brown arrow) is transferred to the charge transport calculation module which provides the drift-diffusion simulation of a device. The results of this calculation are processed by the last unit which performs the plotting of the voltage-current curve, the charge carriers and field distributions.

As an example we present the results for a single calculation of this chain for α -NPD material. On the first stage we obtained the microstructure of the material with the average density $\rho = 1.16 \text{ g/cm}^3$ (experimentally estimated value is 1.19 g/cm^3 (28)), the average distance between the centers of molecules is 5.9 \AA . On the second stage we calculated the density of states $g(E)$ for electrons and holes in the bulk material and defined HOMO and LUMO energies and disorder parameters: $E_{LUMO} = -1.24 \text{ eV}$, $\sigma_e = 0.07 \text{ eV}$, $E_{HOMO} = -5.18 \text{ eV}$, $\sigma_h = 0.1 \text{ eV}$. These material parameters were used in the drift-diffusion simulations together with the mobility values estimated in the experiment. As electrodes we used PEDOT:PSS ($W = 5.15 \text{ eV}$) and ITO ($W = 5.05 \text{ eV}$). The plots of the current-voltage curve $J(V)$ and carrier densities along the device $n(x)$ for electrons and $p(x)$ for holes as displayed in the platform interface are shown in **Figure 5**.

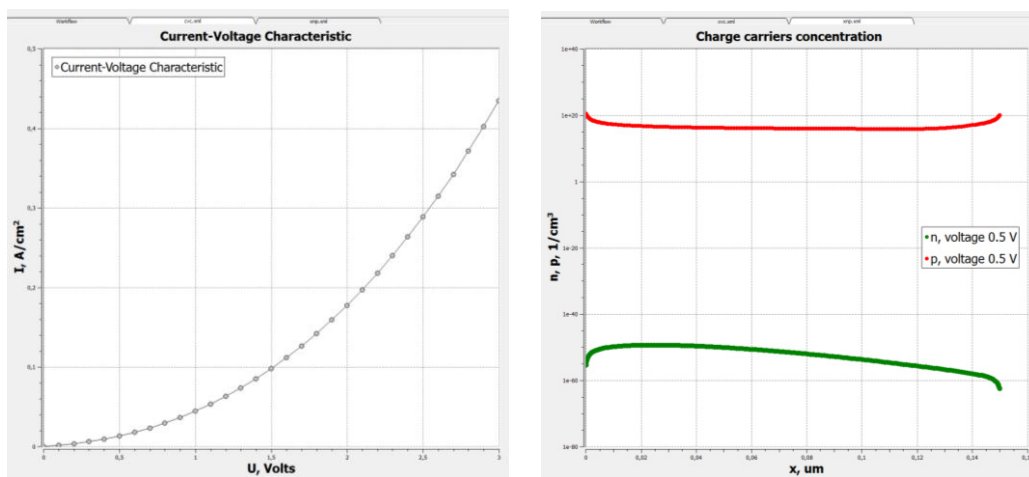


Figure 5 Voltage-current curve (left) and carriers' concentration distribution along the device (right).

In the single-carrier (hole only) device the electron concentrations are negligible as expected. The current-voltage curve is the macroscopic characteristics of the device that may be directly used for comparison with the experiment. Charge densities inside the layer can usually be not measured experimentally, but their analysis allows one to understand the charge transfer mechanisms and limitations predicted by the model.

8 Conclusions and Future Work

In this work we presented a simulation platform which serves as an integrated framework for multiscale and multiphysics modeling of Organic Light Emitting Diodes (OLEDs) and their components. This product is aimed to provide and facilitate several aspects of scientific work which are listed below.

Numerical simulation: the platform includes different numerical methods to calculate atomistic properties of organic molecules, organic layer microstructure and energy properties of layers, charge carrier and excitation transport and kinetics, optical properties of multilayer devices and integrated properties of a device;

Task management: ability to work with remote high performance computing (HPC) resources, and to manage multiple independent parallel tasks;

Data exchange and data storage: automatic data exchange between different physical models, data storage in a dedicated database;

Graphical user interface: desktop with different computational modules and blocks provides an obvious way to construct computational chains. Starting from constructing an arbitrary OLED device and specifying its properties, one can combine modules at different scales in a variety of flexible computational chains, aimed at the full characterization of the considered OLED device, from the atomistic level, through transport and optical properties to the integral device characteristics.

In summary, the proposed platform is a powerful tool for the predictive modeling and design of OLEDs and their components.

The future work will be focused on the validation of complex computational chains featuring several physical levels; sensitivity analysis of OLED device properties with respect to different material parameters at atomistic and mesoscopic level; development of optimization tools for arbitrary figures of merit (device efficiency etc.); development and integration of various computational methods, including parameter fitting, extending the set of available simulation tools.

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